

STIC Search Report Biotech-Chem Library

STIC Database Tracking Marriage

TO: Ben Sackey

Location: 5b31 / 5c18

Art Unit: 1626

Thursday, October 13, 2005

Case Serial Number: 10/611539

From: Noble Jarrell

Location: Biotech-Chem Library

Rem 1B71

Phone: 272-2556

Noble.jarrell@uspto.gov

Search Notes	
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PTO-1590 (8-01)

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: BEN SACKEY Examiner #: 73489 Date: 10/7/05 Art Unit: 1636 Phone Number 302-0705 Serial Number: 10/6/1, 539 Mail Box and Bldg/Room Location: 16m 583/Results Format Preferred (circle): PAPER DISK E-MAIL							
If more than one search is submitted, please prioritize searches in order of need.							

Title of Invention: Inhibitors of Cyclin Dependent kings es of their uses Inventors (please provide full names): fal at al.							
Inventors (please provide full names):	fal et	al.					
Earliest Priority Filing Date:	119/02.						
For Sequence Searches Only Please inclu	de all pertinent information	(parent, child, divisional, or issued patent numbers) along with the					
appropriate serial number.		a line in a claim I Accin C	en o				
Sub:	stituents on	2 as de pried in commissions	,				
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appropriate serial number. Substituents are as defined in claim I this case by the tree restricted and the Elected compet is the last the seem restricted and the Elected compet is Example 11, which is ((+)-lans-2-(2-Chlauphengl)-5,7- are dihydroxymethyd-1-methyl pywrolidin-3-71) chromen-4-							
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Date Searcher Picked Up: 10/13/05	Structure (#)	Questel/Orbit					
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(FILE 'HOME' ENTERED AT 11:06:49 ON 13 OCT 2005)

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- 1 US2004106581/PN OR (US2003-611539# OR US2002-397326#)/AP,PRN L1
- L21 IN2002-MU616#/AP, PRN
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This file contains CAS Registry Numbers for easy and accurate substance identification.

- ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN T.3
- 2004:41203 HCAPLUS AN
- DN 140:111277
- ED Entered STN: 18 Jan 2004
- TI Preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent
- IN Lal, Bansi; Joshi, Kalpana Sanjay; Kulkarni, Sanjeev Anant; Mascarenhas, Malcolm; Kamble, Shrikant Gangadhar; Rathos, Maggie Joyce; Joshi, Rajendrakumar Dinanath
- Nicholas Piramal India Limited, India PCT Int. Appl., 186 pp. PΑ
- SO

CODEN: PIXXD2

- DT Patent
- LA English
- IC ICM A61K
- CC 27-14 (Heterocyclic Compounds (One Hetero Atom)) Section cross-reference(s): 1, 5, 63

FAN.CNT 1

PATENT NO. DATE KIND DATE APPLICATION NO.

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Title compds. [I; R1 = (substituted) aryl, (unsatd.) heterocyclyl, NR9R10, AΒ OR11, SR11; R2 = H, alkyl, (substituted) aryl, (unsatd.) heterocyclyl, OR11, halo, cyano, NO2, NR9R10, SR11; R3-R5 = H, alkyl, halo, OR11, aralkoxy, alkylcarbonyloxy, CO2H, NR9R10, SR11, aralkylthio, alkylsulfonyl, arylsulfonyl, SO2NR9R10, aryl, (unsubstituted) heterocyclyl, etc.; R6 = alkyleneOR11; R8 = H, alkyl, aryl, carboxamide, sulfonamide, NR9R10, OR11; R9, R10 = H, alkyl, aryl, alkanoyl, heterocyclyl, etc.; NR9R10 = (unsatd.) (substituted) heterocyclyl; R11 = H, alkyl, alkanoyl, (substituted) aryl; Z = O, S, NR8; A = 5-7 membered ring], were prepared Thus, trans-2-(2-chloro-5-fluorophenyl)-5,7-dihydroxy-8-(2-hydroxymethyl-1-methylpyrrolidin-3-yl)chromen-4-one (preparation given) inhibited HeLa cervix cell proliferation with IC50 = $0.01-1 \mu M$. pyrrolidinylchromenone prepn cyclin dependent kinase inhibitor; anticancer ST antifungal antiviral parasiticide insecticide chromenone pyrrolidinyl prepn

```
IT
     Cyclins
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (D1, inhibitors; preparation of pyrrolidinylchromenones as inhibitors of
        cyclin-dependent kinases)
IT
    Cyclins
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (E, inhibitors; preparation of pyrrolidinylchromenones as inhibitors of
        cyclin-dependent kinases)
    Disease, animal
IT
        (degenerative, treatment; preparation of pyrrolidinylchromenones as
        inhibitors of cyclin-dependent kinases)
ΙT
    Agriculture and Agricultural chemistry
     Antitumor agents
     Fungicides
    Human
     Insecticides
     Parasiticides
        (preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent
        kinases)
TT
    Disease, animal
        (proliferative, treatment; preparation of pyrrolidinylchromenones as
        inhibitors of cyclin-dependent kinases)
    Antiviral agents
TТ
     Kidney, disease
     Mycosis
     Neoplasm
     Skin, disease
        (treatment; preparation of pyrrolidinylchromenones as inhibitors of
        cyclin-dependent kinases)
IT
     Infection
        (viral, treatment; preparation of pyrrolidinylchromenones as inhibitors of
        cyclin-dependent kinases)
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     141349-86-2, Cyclin dependent kinase-2
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                150428-23-2, Cyclin-dependent kinase
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     (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic
     use); BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

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(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
         (preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent
        kinases)
IT
     117955-09-6P
     RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic
     preparation); PREP (Preparation); RACT (Reactant or reagent)
         (preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent
        kinases)
IT
     62-23-7, 4-Nitrobenzoic acid
                                   88-65-3, 2-Bromobenzoic acid
                                                                   93-58-3,
     Methyl benzoate 99-60-5, 2-Chloro-4-nitrobenzoic acid 104-94-9, 4-Methoxyaniline 106-94-5, n-Propyl bromide 118-91-2, 2-Chlorobenzoic
           394-35-4, Methyl 2-fluorobenzoate 455-68-5, Methyl
     3-fluorobenzoate 606-45-1, 2-Methoxybenzoic acid methyl ester
     610-94-6, Methyl 2-bromobenzoate 610-96-8, Methyl 2-chlorobenzoate
     610-97-9, Methyl 2-iodobenzoate 619-42-1, Methyl 4-bromobenzoate
     621-23-8, 1,3,5-Trimethoxybenzene 785-56-8, 3,5-
     Bis(trifluoromethyl)benzoyl chloride 1129-35-7, Methyl 4-cyanobenzoate
     1445-73-4, 1-Methyl-4-piperidone 2810-04-0, Thiophene-2-carboxylic acid
     ethyl ester
                  2905-65-9, Methyl 3-chlorobenzoate
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     4-trifluoromethylbenzoate 16220-95-4, Methyl 2-chloro-5-methylbenzoate
     18063-02-0, 2,6-Difluoro-1-benzoyl chloride 27007-53-0, Methyl
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               220389-17-3, Ethyl 2-methyl-4-cyanobenzoate 647020-69-7
     647020-70-0, Methyl 2-Chloro-3-fluorobenzoate
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     2-bromo-3-fluorobenzoate
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent
        kinases)
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C07D405-02; C07D405-14

WO2004004632 A UPAB: 20040318 NOVELTY - Benzopyranone derivatives (Ic) and their prodrug, tautomeric form, stereo isomer, optical isomer, pharmaceutically acceptable salt, pharmaceutically acceptable solvate or polymorphs are new. DETAILED DESCRIPTION - Benzopyranone derivatives of formula (Ic) and their prodrug, tautomeric form, stereoisomer, optical isomer, pharmaceutically acceptable salt, pharmaceutically acceptable solvate or polymorphs are new. R1 = aryl (optionally substituted with T) optionally saturated or 1-4C heterocycle having hetero atoms of N, O, S or P (optionally substituted with T), NR9R10, OR11 or SR11; R2 = H, 1-6C alkyl, aryl (optionally substituted with T), optionally saturated or 1-4C heterocycle having heteroatoms of N, O, S or P (optionally substituted with T), OR11, halo, CN, NO2, NR9R10 or SR11; R3, R4, R5 = H, 1-6C-alkyl, halo, OR11, aryl1-4C-alkoxy, 1-4C-alkylcarbonyloxy, 1-4C-alkoxycarbonyloxy, arylcarbonyloxy, carboxy, CN, NO2 NR9R10, SR11, aryl-1-4C-alkylthio, SO2-1-4C-alkyl, SO2-aryl, SO2NR9R10, aryl and 1-4C heterocycle identical or different heteroatoms of N, O, S or P; R6 = 1-4C-alkyleneOR11; Z = O, S or NR8; A = 5-7 membered ring; and $T = halo, 1-4C \ alkyl, 1-4c \ alkoxy, 2-6C \ alkenyl, 3-6C \ alkynyl, 2-4C$ alkanoyl, NO2, NR9R10, SR-11, CF3, hydroxyl, CN, carboxy, 1-4C alkoxy carbonyl or 1-4C alkylenehydroxyl. INDEPENDENT CLAIMS also included for (1) benzopyranone derivatives of formula (Ig); (2) preparation of (Ic) or (Ig). (3) preparation of benzopyranone derivatives of formula (XIIIA), (XXXIA) and (XXXVII); and (4) resolution of anisole derivatives of formula (VIIIA). R1 = aryl (optionally substituted with T) optionally saturated or 1-4C heterocycle having hetero atoms of N, O, S or P (optionally substituted with T), NR9R10, OR11 or SR11; R2 = H, 1-6C alkyl, aryl (optionally substituted with T), optionally saturated or 1-4C heterocycle having heteroatoms of N, O, S or P (optionally substituted with T), OR11, halo, CN, NO2, NR9R10 or SR11; R3, R4, R5 = H, 1-6C-alkyl, halo, OR11, aryl1-4C-alkoxy, 1-4C-alkylcarbonyloxy, 1-4C-alkoxycarbonyloxy, arylcarbonyloxy, carboxy, CN, NO2 NR9R10, SR11, aryl-1-4C-alkylthio, SO2-1-4C-alkyl, SO2-aryl, SO2NR9R10, aryl and 1-4C heterocycle identical or different heteroatoms of N, O, S or P; R6 = 1-4C-alkyleneOR11; Z = 0, S or NR8; A = 5-7 membered ring; $T = halo, 1-4C \ alkyl, 1-4c \ alkoxy, 2-6C \ alkenyl, 3-6C \ alkynyl, 2-4C$ alkanoyl, NO2, NR9R10, SR-11, CF3, hydroxyl, CN, carboxy, 1-4C alkoxy carbonyl or 1-4C alkylenehydroxyl; and R13 = H, 1-6C-alkyl, (optionally substituted with halo, OH, carboxyl, 1-4C-alkoxy, amino, NO2, 1-4C-alkylthio, sulfhydryl or sulfonyl), 2-6C-alkenyl (optionally substituted with halo, OH, carboxyl, 1-4C-alkoxy, NH2, NH2, 1-4C-alkylthio, sulfhydryl, sulfonyl) aryl (optionally substituted with T, OH, 1-4C-alkoxy, 1-4C-alkylcarbonyl, CN, SO2R10, CO-(CH2)m-R14). Full definitions are given in the DEFINITIONS (Full Definitions) field.

ACTIVITY - Cytostatic; Nephrotropic; Insecticide; Virucide;

Antiparasitic; Antimicrobial; Dermatological.

(+)-trans-2-(2-Bromo-phenyl)-5,7-dihydroxy-8-(2-hydroxymethyl-1-methyl-pyrrolidin-3-yl)-chromen-4-one (I'c) was assessed for its

methyl-pyrrolidin-3-yl)-chromen-4-one (I'c) was assessed for its inhibitory action using in vitro cell proliferation assay in human cancerous cell lines (PC-3 Prostate (a), H-460 Lung (b), MDA-MB-231 Breast (c), MCF-7 Breast (d), HeLa Cervix (e) and U-937 Histiocytic Lymphoma (f) (monocytes)).

The median inhibitory concentration values of (I'c) for (a)-(f) were 0.1-1, 0.5-1, 1-10, 0.1, greater than 10 and 0.1-1, respectively.

```
MECHANISM OF ACTION - Cyclin dependent kinase inhibitor
          USE - Compounds (Ic)/(Ig) are useful in the manufacture of a
     medicament for the inhibition of cyclin-dependent kinases, for the
     treatment or prevention of proliferative disorders associated with
     de-differentiation of a differentiated cell population in a mammal, for
     the treatment or prevention of disorders associated with excessive cell
     proliferation, cancer, degenerative disorders, mycotic infections, viral
     infections, parasitic diseases, dermatological disorders or nephrological
     disorders, and as an insecticide or in agricultural applications.
     (claimed)
          ADVANTAGE - Compounds (Ic)/(Ig) have enhanced selectivity and low
     cytotoxicity.
     Dwg.0/0
FS
     CPI
FA
     AB; GI; DCN
MC
     CPI: B05-B01E; B06-A01; B07-H; B14-A02; B14-A04; B14-B02; B14-B04B;
          B14-D06; B14-H01; B14-N10; B14-N17; C05-B01E; C06-A01; C07-H; C14-A02; C14-A04; C14-B02; C14-B04B; C14-D06; C14-H01; C14-N10;
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L6
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L8
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L9
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L10
                SAV TEM L10 SAC539F0/A
L11
                STR L8
L12
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L15
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T.18
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L19
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L20
           1438 E3-20
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              5 E13-16
L21
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L22
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L23
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L24
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                E RATHOS M/AU
L25
              2 E4-5
                E JOSHI R/AU
            532 E3-18, E32-34, E36
L26
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L27
           1652 E3-4
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L28
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L29
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L31
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E CYCLIN DEPEND/CT
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L32
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                E E29+ALL
                E E2+ALL
T<sub>4</sub>3.3
           5876 CYCLIN-DEPENDENT PROTEIN KINASE+NT/CT
L34
           9069 L31
L35
            188 L30 AND L32-34
            181 L35 AND INHIBIT?
L36
L37
             49 L32 AND L30
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L38
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L42
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L43
L44
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L45 '
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1.46
L47
              5 L45 FULL SUB=L13
                SAV TEM L47 SAC539S1/A
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L50
            796 OSC3/ES
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L51
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L52
L53
            195 L49, L52
L54
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             82 L53 NOT L54
L55
L56
                STR L11
L57
              8 L56 SAM SUB=L53
T<sub>1</sub>5.8
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L59
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L60
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L61
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L62
             14 L59-60 NOT L61-62
L63
L64
              1 L61-62
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L66
              3 L65
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```

STRUCTURE FILE UPDATES: 12 OCT 2005 HIGHEST RN 865114-63-2 DICTIONARY FILE UPDATES: 12 OCT 2005 HIGHEST RN 865114-63-2

provided by InfoChem.

Property values tagged with IC are from the ZIC/VINITI data file

New CAS Information Use Policies, enter HELP USAGETERMS for details.

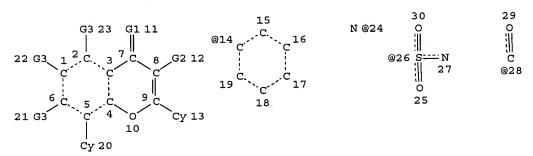
TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html





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VAR G2=H/AK/14
VAR G3=H/AK/X/31/24/26/28/CN/NO2/OH/34
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

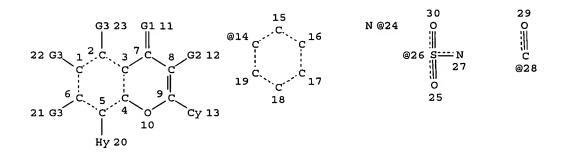
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RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE

L10 1179 SEA FILE=REGISTRY SSS FUL L8
L11 STR

Search done by Noble Jarrell



VAR G1=O/S
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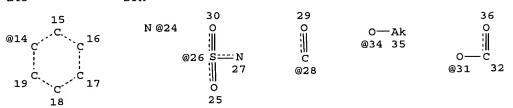
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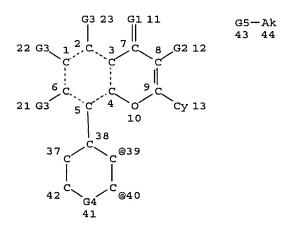
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VAR G4=O/N/S

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NODE ATTRIBUTES:

NSPEC IS RC AT 24

NSPEC IS RC AT 27

DEFAULT MLEVEL IS ATOM

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STEREO ATTRIBUTES: NONE

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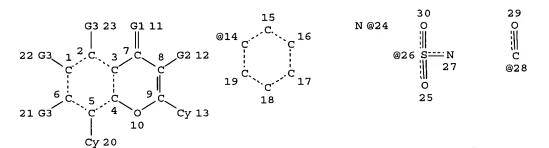
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5 ANSWERS

SEARCH TIME: 00.00.01

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VAR G2=H/AK/14

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NSPEC IS RC AT 27

DEFAULT MLEVEL IS ATOM

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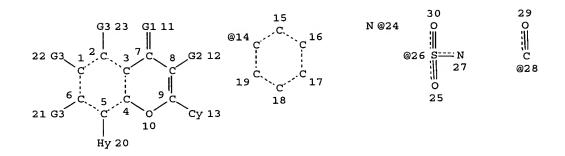
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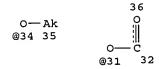
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L10 1179 SEA FILE=REGISTRY SSS FUL L8

L11 STR





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NSPEC IS RC AT 24 NSPEC IS RC AT 27 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE

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VAR G4=O/N/S
VAR G5=39/40
NODE ATTRIBUTES:
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NSPEC IS RC AT 27
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE

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L48 888 SEA FILE=REGISTRY ABB=ON PLU=ON L13 NOT L47

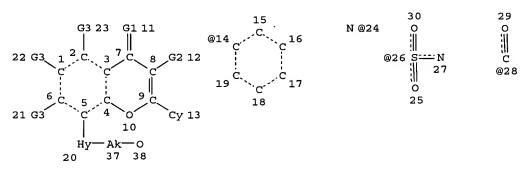
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OR OSC3)/ES

L52 14 SEA FILE=REGISTRY ABB=ON PLU=ON (NCNC2 OR NCOC2 OR NCSC2 OR OCOC2 OR NCOC2 OR OCSC2)/ES AND L48

L53 195 SEA FILE=REGISTRY ABB=ON PLU=ON (L49 OR L52)

L56 STR





VAR G1=O/S
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VAR G3=H/AK/X/31/24/26/28/CN/NO2/OH/34
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NSPEC IS RC AT 24
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GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 37

STEREO ATTRIBUTES: NONE

DEFAULT ECLEVEL IS LIMITED

L58 111 SEA FILE=REGISTRY SUB=L53 SSS FUL L56

100.0% PROCESSED 186 ITERATIONS 111 ANSWERS

SEARCH TIME: 00.00.01

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L64 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN
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- AN 2004:41203 HCAPLUS
- DN 140:111277
- ED Entered STN: 18 Jan 2004
- TI Preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent kinases.
- IN Lal, Bansi; Joshi, Kalpana Sanjay; Kulkarni, Sanjeev Anant; Mascarenhas, Malcolm; Kamble, Shrikant Gangadhar; Rathos, Maggie Joyce; Joshi, Rajendrakumar Dinanath
- PA Nicholas Piramal India Limited, India
- SO PCT Int. Appl., 186 pp.
- CODEN: PIXXD2
 DT Patent
- LA English
- IC ICM A61K
- CC 27-14 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 5, 63

FAN.CNT 1

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PI	WO 2004004632	A2 20040115	WO 2003-IN234	20030707 <
	WO 2004004632	A3 20040916		
	WO 2004004632	C1 20050324		
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	LS, LT, LU	, LV, MA, MD, MG,	MK, MN, MW, MX, MZ, NI	, NO, NZ, OM,
	PG, PH, PL	, PT, RO, RU, SC,	SD, SE, SG, SK, SL, SY,	, TJ, TM, TN,
	TR, TT, TZ	, UA, UG, US, UZ,	VC, VN, YU, ZA, ZM, ZW	•
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	FI, FR, GB	, GR, HU, IE, IT,	LU, MC, NL, PT, RO, SE,	, SI, SK, TR,
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EP 1556375
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                        C07D405/14+311C+233+207
os
     MARPAT 140:111277
GT
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Insecticides Parasiticides

AB

I

OR11, SR11; R2 = H, alkyl, (substituted) aryl, (unsatd.) heterocyclyl, OR11, halo, cyano, NO2, NR9R10, SR11; R3-R5 = H, alkyl, halo, OR11, aralkoxy, alkylcarbonyloxy, CO2H, NR9R10, SR11, aralkylthio, alkylsulfonyl, arylsulfonyl, SO2NR9R10, aryl, (unsubstituted) heterocyclyl, etc.; R6 = alkyleneOR11; R8 = H, alkyl, aryl, carboxamide, sulfonamide, NR9R10, OR11; R9, R10 = H, alkyl, aryl, alkanoyl, heterocyclyl, etc.; NR9R10 = (unsatd.) (substituted) heterocyclyl; R11 = H, alkyl, alkanoyl, (substituted) aryl; Z = O, S, NR8; A = 5-7 membered ring], were prepared Thus, trans-2-(2-chloro-5-fluorophenyl)-5,7-dihydroxy-8-(2-hydroxymethyl-1-methylpyrrolidin-3-yl)chromen-4-one (preparation given) inhibited HeLa cervix cell proliferation with IC50 = 0.01-1 μM . stpyrrolidinylchromenone prepn cyclin dependent kinase inhibitor; anticancer antifungal antiviral parasiticide insecticide chromenone pyrrolidinyl prepn IT Cvclins RL: BSU (Biological study, unclassified); BIOL (Biological study) (D1, inhibitors; preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent kinases) IT RL: BSU (Biological study, unclassified); BIOL (Biological study) (E, inhibitors; preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent kinases) IT Disease, animal (degenerative, treatment; preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent kinases) IT Agriculture and Agricultural chemistry Antitumor agents Fungicides Human

Title compds. [I; R1 = (substituted) aryl, (unsatd.) heterocyclyl, NR9R10,

(preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent

```
kinases)
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        (proliferative, treatment; preparation of pyrrolidinylchromenones as
        inhibitors of cyclin-dependent kinases)
IT
     Antiviral agents
     Kidney, disease
    Mycosis
     Neoplasm
     Skin, disease
        (treatment; preparation of pyrrolidinylchromenones as inhibitors of
        cyclin-dependent kinases)
TΤ
     Infection
        (viral, treatment; preparation of pyrrolidinylchromenones as inhibitors of
        cyclin-dependent kinases)
TТ
     141349-86-2, Cyclin dependent kinase-2
                                              147014-97-9, Cyclin dependent
               150428-23-2, Cyclin-dependent kinase
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (inhibitors; preparation of pyrrolidinylchromenones as inhibitors of
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     647019-62-3P 647019-63-4P 647019-64-5P
     647019-65-6P 647019-66-7P 647019-67-8P
     647019-68-9P 647019-69-0P 647019-70-3P
     647019-71-4P 647019-72-5P 647019-73-6P
     647019-74-7P 647019-75-8P 647019-76-9P
     647019-77-0P 647019-78-1P 647019-79-2P
     647019-81-6P 647019-82-7P 647019-84-9P
     647019-85-0P 647019-86-1P 647019-87-2P
     647019-88-3P 647019-89-4P 647019-90-7P
     647019-91-8P 647019-92-9P 647019-93-0P
     647019-94-1P 647019-95-2P 647019-96-3P
     647019-97-4P 647019-98-5P 647019-99-6P
     647020-00-6P 647020-01-7P 647020-02-8P
     647020-03-9P 647020-04-0P 647020-05-1P
     647020-06-2P 647020-07-3P 647020-08-4P
                    647020-10-8P
                                   647020-11-9P
                                                   647020-12-0P
     647020-09-5P
                   647020-14-2P
                                   647020-15-3P
                                                   647020-16-4P
                                                                  647020-17-5P
     647020-13-1P
     647020-18-6P 647020-19-7P 647020-20-0P
     647020-21-1P 647020-22-2P 647020-23-3P
     647020-24-4P 647020-25-5P 647020-26-6P
     647020-27-7P 647020-28-8P 647020-29-9P
     647020-30-2P 647020-31-3P 647020-32-4P
     647020-33-5P 647020-34-6P 647020-35-7P
     647020-36-8P 647020-37-9P 647020-38-0P
     647020-39-1P 647020-40-4P 647020-41-5P
     647020-42-6P 647020-43-7P 647020-44-8P
     647020-46-0P 647020-47-1P 647020-48-2P
     647020-49-3P 647020-50-6P 647020-51-7P
     647020-52-8P 647020-53-9P 647020-54-0P
     647020-55-1P 647020-56-2P 647020-57-3P
     647020-58-4P
     RL: AGR (Agricultural use); BSU (Biological study, unclassified); PAC
     (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic
     use); BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent
        kinases)
ΙT
     647020-75-5P 647020-76-6P 647020-77-7P
     647020-78-8P 647020-80-2P 647020-81-3P
                                   647020-84-6P
                                                   647020-85-7P
                    647020-83-5P
     647020-82-4P
     647020-86-8P
                    647020-87-9P
                                   647020-88-0P 647020-89-1P
     647020-90-4P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
```

```
(preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent
       kinases)
IT
    117955-09-6P
    RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic
    preparation); PREP (Preparation); RACT (Reactant or reagent)
        (preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent
       kinases)
                                   88-65-3, 2-Bromobenzoic acid
IT
    62-23-7. 4-Nitrobenzoic acid
                                                            104-94-9,
    Methyl benzoate
                     99-60-5, 2-Chloro-4-nitrobenzoic acid
                      106-94-5, n-Propyl bromide 118-91-2, 2-Chlorobenzoic
    4-Methoxyaniline
          394-35-4, Methyl 2-fluorobenzoate 455-68-5, Methyl
    3-fluorobenzoate 606-45-1, 2-Methoxybenzoic acid methyl ester
    610-94-6, Methyl 2-bromobenzoate 610-96-8, Methyl 2-chlorobenzoate
    610-97-9, Methyl 2-iodobenzoate 619-42-1, Methyl 4-bromobenzoate
    621-23-8, 1,3,5-Trimethoxybenzene
                                       785-56-8, 3,5-
    Bis(trifluoromethyl)benzoyl chloride 1129-35-7, Methyl 4-cyanobenzoate
    1445-73-4, 1-Methyl-4-piperidone 2810-04-0, Thiophene-2-carboxylic acid
                 2905-65-9, Methyl 3-chlorobenzoate
    ethyl ester
                                                      2942-59-8,
    2-Chloro-3-pyridinecarboxylic acid 2967-66-0, Methyl
    4-trifluoromethylbenzoate 16220-95-4, Methyl 2-chloro-5-methylbenzoate
    18063-02-0, 2,6-Difluoro-1-benzoyl chloride 27007-53-0, Methyl
    2-Bromo-5-chlorobenzoate 86393-34-2, 2,4-Dichloro-5-fluorobenzoyl
    chloride
              220389-17-3, Ethyl 2-methyl-4-cyanobenzoate
                                                           647020-69-7
    647020-70-0, Methyl 2-Chloro-3-fluorobenzoate
                                                   647020-71-1, Methyl
    2-bromo-3-fluorobenzoate
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent
       kinases)
IT
    943-14-6P, 2-Bromo-5-nitrobenzoic acid
                                             2516-96-3P, 2-Chloro-5-
    nitrobenzoic acid 6307-82-0P, 2-Chloro-5-nitrobenzoic acid methyl ester
    6942-37-6P, 5-Amino-2-bromobenzoic acid methyl ester
                                                          13296-94-1P,
    2-Bromo-4-nitroaniline 13324-11-3P, 2-Chloro-4-nitrobenzoic acid methyl
           16426-64-5P, 2-Bromo-4-nitrobenzoic acid 34662-35-6P,
    2-Bromo-4-nitrobenzonitrile 35450-36-3P, 2-Bromo-5-methoxybenzoic acid
    methyl ester 42122-75-8P, 5-Amino-2-chlorobenzoic acid methyl ester
    46004-37-9P, 4-Amino-2-chlorobenzoic acid methyl ester 54810-63-8P,
    2-Chloro-5-methoxybenzoic acid methyl ester 74317-85-4P,
    2-Bromo-4-methoxybenzoic acid
                                   94635-24-2P, 1-(4-Methoxyphenyl)-4-
                98592-34-8P, 2-Chloro-4-cyanobenzoic acid methyl ester
    piperidone
    104253-44-3P, 2-Chloro-4-hydroxybenzoic acid methyl ester
                                                                104253-45-4P,
                                                 113225-07-3P
    2-Chloro-4-methoxybenzoic acid methyl ester
                                                                 113225-08-4P
    137548-16-4P, 2-Chloro-5-dimethylaminobenzoic acid methyl ester
    154607-00-8P, 2-Bromo-5-hydroxybenzoic acid methyl ester
                                                               185312-82-7P,
    4-Bromo-2-chlorobenzoic acid methyl ester 217458-79-2P
                                                               247092-10-0P,
    2-Chloro-5-hydroxybenzoic acid methyl ester 647020-59-5P 647020-60-8P
                                  647020-63-1P, 2-Chloro-5-fluorobenzoic acid
                  647020-62-0P
     647020-61-9P
                                  647020-65-3P, 1-(4-Methoxyphenyl)-4-(2,4,6-
    methyl ester
                   647020-64-2P
    trimethoxyphenyl)-1,2,3,6-tetrahydropyridine 647020-66-4P
                                                                  647020-67-5P
                                                 647020-74-4P
     647020-68-6P
                  647020-72-2P
                                  647020-73-3P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent
       kinases)
     647019-53-2P
    RL: AGR (Agricultural use); BSU (Biological study, unclassified); PAC
     (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic
     use); BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent
       kinases)
RN
     647019-53-2 HCAPLUS
    4H-1-Benzopyran-4-one, 2-(2-chlorophenyl)-8-[(2R,3S)-2-(hydroxymethyl)-1-
CN
    methyl-3-pyrrolidinyl]-5,7-dimethoxy-, rel- (9CI) (CA INDEX NAME)
```

Relative stereochemistry.

```
=> d all hitstr 163 tot
    ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
L63
AN
     2003:297263 HCAPLUS
     139:348048
DN
     Entered STN: 17 Apr 2003
ED
     C-glucoside flavonoids from the leaves of Crataegus pinnatifida Bge. var.
ΤI
     major N.E.Br.
     Zhang, Pei-Cheng; Xu, Sui-Xu
AU
     Inst. Materia Med., Peking Union Med. College, Chinese Acad. Med. Sci.,
CS
     Beijing, 100050, Peop. Rep. China
so
     Journal of Asian Natural Products Research (2003), 5(2), 131-136
     CODEN: JANRFI; ISSN: 1028-6020
PR
     Taylor & Francis Ltd.
DT
     Journal
LΑ
     English
CC
     11-1 (Plant Biochemistry)
AΒ
     Two new acetyl C-glucoside flavonoids, 8-C-β-d-(2''-O-
     acetyl)glucofuranosylapigenin and 3''-O-acetylvitexin, along with 4 known
     C-glucoside flavonoids, vitexin, 6''-O-acetylvitexin, 2''-O-acetylvitexin,
     and 2''-O-rhamnosylvitexin were isolated from the leaves of Crataegus
     pinnatifida Bge. var. major N.E.Br. Their structures were elucidated by
     spectroscopic means and chemical evidence.
     C glucoside flavonoid Crataegus
ST
IT
     New natural products
        (8-C-β-d-(2''-O-acetyl)glucofuranosylapigenin and
        3''-O-acetylvitexin (C-glucoside flavonoids))
IT
     Crataegus pinnatifida
        (C-glucoside flavonoids from the leaves of Crataegus pinnatifida)
IT
     Flavonoids
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (C-glucoside flavonoids from the leaves of Crataegus pinnatifida)
IT
     Molecular structure, natural product
        (of 8-C-β-d-(2''-O-acetyl)glucofuranosylapigenin and
        3''-O-acetylvitexin (C-glucoside flavonoids))
                          64820-99-1, 2''-O-Rhamnosylvitexin
                                                                156790-77-1,
IT
     3681-93-4, Vitexin
     6''-O-Acetylvitexin
                          264142-91-8
     RL: BSU (Biological study, unclassified); PRP (Properties); BIOL
     (Biological study)
        (C-glucoside flavonoids from the leaves of Crataegus pinnatifida)
IT
     439692-84-9
                   439692-86-1
     RL: BSU (Biological study, unclassified); PRP (Properties); BIOL
     (Biological study)
        (new C-glucoside flavonoids from the leaves of Crataegus pinnatifida)
RE.CNT
              THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
       10
RE
(1) Ammon, H; Planta Med 1981, V43, P209 HCAPLUS
```

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(2) Chen, H; J Chin Mater Med 1994, V19(8), P454 MEDLINE
(3) Dauguet, J; Phytochemistry 1993, V33(6), P1503 HCAPLUS
(4) Fang, Y; Chin Trad Herbal Drugs 1982, V13(5), P26 HCAPLUS
(5) Kashnikova, M; Khim Prir Soedin 1984, V1, P108
(6) Lin, L; J Chin Pharm University 1999, V30(1), P21 HCAPLUS
(7) Nikolov, N; Planta Med 1982, V44, P50 HCAPLUS
(8) Yang, L; Chin Trad Herbal Drugs 1993, V24(9), P482
(9) Zhang, P; J Asian Nat Prod Res 2001, V3(1), P77 HCAPLUS
(10) Zhang, P; Phytochemistry 2001, V57, P1249 HCAPLUS
     439692-84-9
     RL: BSU (Biological study, unclassified); PRP (Properties); BIOL
     (Biological study)
        (new C-glucoside flavonoids from the leaves of Crataegus pinnatifida)
RN
     439692-84-9 HCAPLUS
     4H-1-Benzopyran-4-one, 8-(2-0-acetyl-β-D-glucofuranosyl)-5,7-
CN
     dihydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)
```

Absolute stereochemistry. Rotation (+).

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ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
L63
AN
     2002:881393 HCAPLUS
DN
     138:119880
     Entered STN: 21 Nov 2002
ED
     Phenolic and flavone C-glycosides from Scleranthus uncinatus
TI
ΑU
     Yayli, Nurettin; Baltaci, Cemalettin; Genc, Hasan; Terzioglu, Salih
     Faculty of Science, Department of Chemistry, Karadeniz Technical
CS
     University, Trabzon, Turk.
     Pharmaceutical Biology (Lisse, Netherlands) (2002), 40(5), 369-373
so
     CODEN: PHBIFC; ISSN: 1388-0209
     Swets & Zeitlinger B.V.
PB
DT
     Journal
LΑ
     English
CC
     11-1 (Plant Biochemistry)
GT
```

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

From the whole parts of Scleranthus uncinatus, a new flavone C-glycoside, 5,7,4'-trihydroxy-3'-methoxyflavone-8-C-β-xylofuranoside-2"-Oglucoside (I), and a maltol phenolic glycoside, 2-methyl-3-0- $\{2'-[\beta-D-glucoside-(1''' \rightarrow 3")-\beta-D-glucoside\}$ -propionyloxy-4'methoxyphenyl}-4-pyrone (II), were isolated for the first time from the S. uncinatus. The structures of I and II were deduced by high field 1D and 2D 400 MHz NMR and (+) FAB-MS spectra.

stglycoside Scleranthus

```
TT
     Glycosides
     RL: BSU (Biological study, unclassified); PRP (Properties); PUR
     (Purification or recovery); BIOL (Biological study); PREP (Preparation)
        (flavonoid, oxo; phenolic and flavone glycosides from Scleranthus
        uncinatus)
IT
     Scleranthus uncinatus
        (phenolic and flavone glycosides from Scleranthus uncinatus)
IT
     Glycosides
     RL: BSU (Biological study, unclassified); PRP (Properties); PUR
     (Purification or recovery); BIOL (Biological study); PREP (Preparation)
        (phenolic; phenolic and flavone glycosides from Scleranthus uncinatus)
IT
     490036-65-2P
                    490036-67-4P
     RL: BSU (Biological study, unclassified); PRP (Properties); PUR
     (Purification or recovery); BIOL (Biological study); PREP (Preparation)
        (phenolic and flavone glycosides from Scleranthus uncinatus)
RE.CNT
              THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Agrawal, P; Carbon-13 NMR offiavonoids 1989
(2) Agrawal, P; Phytochemistry 1992, V31, P3307 HCAPLUS
(3) Amri, B; Phytochemistry 1991, V30, P3840
(4) Chopin, J; The Flavonoids 1988, P63 HCAPLUS
(5) Davis, P; Flora of Turkey and the East Aegean Islands 1967, V2
(6) Gluchoff-Fiasson, K; Phytochemistry 1989, V28, P2471 HCAPLUS
(7) Harborne, J; The Flavonoids 1988
(8) Hatano, T; Phytochemistry 1999, V52, P1379 HCAPLUS
(9) Krauze-Baranowska, M; Phytochemistry 1995, V39, P727 HCAPLUS
(10) Kuo, S; Phytochemistry 1996, V41, P309 HCAPLUS
(11) Maatooq, G; Phytochemistry 1997, V44, P187 HCAPLUS
(12) Markham, K; Recent Advances in Flavonoid Research 1982, P40
(13) Merghern, R; Phytochemistry 1995, V38, P637
(14) Numata, A; Chem Pharm Bull 1990, V38, P2862 HCAPLUS
(15) Pauli, G; Phytochemistry 1995, V38, P1245 HCAPLUS
(16) Wu, J; Phytochemistry 1997, V45, P1727 HCAPLUS
(17) Yayh, N; Phytochemistry 2001, V58, P607
     490036-65-2P
     RL: BSU (Biological study, unclassified); PRP (Properties); PUR
     (Purification or recovery); BIOL (Biological study); PREP (Preparation)
        (phenolic and flavone glycosides from Scleranthus uncinatus)
RN
     490036-65-2 HCAPLUS
CN
     4H-1-Benzopyran-4-one, 8-(2-O-\beta-D-glucopyranosyl-\beta-D-
     xylofuranosyl)-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)- (9CI)
     INDEX NAME)
```

Absolute stereochemistry. Rotation (-).

L63 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

2002:346522 HCAPLUS AN DN 137:60300 ED Entered STN: 09 May 2002 Two new C-glucoside flavonoids from leaves of Crataegus pinnatifida Bge. TI var. major N. E. Br. AU Zhang, Pei Cheng; Xu, Sui Xu CS Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, 100050, Peop. Rep. China SO Chinese Chemical Letters (2002), 13(4), 337-340 CODEN: CCLEE7; ISSN: 1001-8417 PB Chinese Chemical Society DT Journal LА English CC 11-1 (Plant Biochemistry) Section cross-reference(s): 33 GI

AB Two new C-glucoside flavonoids, namely 8-C-β-D-(2''-O-acetyl)glucofuranosyl apigenin (e.g. I) and 3''-O-acetylvitexin, were isolated from leaves of Crataegus pinnatifida Bge. var. major N. E. Br. Their structures were elucidated by the spectroscopic means and chemical evidence.

Ι

ST flavonoid C glucoside Crataegus

IT Glycosides

RL: NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(C-flavonoid oxo; C-glucoside flavonoids from Crataegus pinnatifida var. major)

IT Crataegus pinnatifida major

New natural products

(C-glucoside flavonoids from Crataegus pinnatifida var. major)

IT Molecular structure, natural product

(of C-glucoside flavonoids from Crataegus pinnatifida var. major)

IT 439692-84-9P 439692-86-1P

RL: NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(C-glucoside flavonoids from Crataegus pinnatifida var. major)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD

- (1) Al Makdessi, H; Arzneim Forsch Drug Res 1996, V46, P25
- (2) Ammon, H; Planta Med 1981, V43, P209 HCAPLUS
- (3) Dauguet, J; Phytochemistry 1993, V33, P1503 HCAPLUS
- (4) Lin, L; J Chin Pharm University 1999, V30, P21 HCAPLUS
- (5) Nikolov, N; Planta Med 1982, V44, P50 HCAPLUS
- (6) Poepping, S; Arzneim Forsch Drug Res 1995, V45(Suppl 2), P1157

IT 439692-84-9P

RL: NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP

Absolute stereochemistry. Rotation (+).

```
L63 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
AN
     2001:128852 HCAPLUS
DN
     134:366704
     Entered STN: 21 Feb 2001
ED
ΤТ
    A stereocontrolled approach to substituted piperidones and piperidines:
     flavopiridol D-ring analogs
    Gross, A.; Borcherding, D. R.; Friedrich, D.; Sabol, J. S.
ΑU
    Aventis Pharmaceuticals Inc., Bridgewater, NJ, 08807-0800, USA
CS
     Tetrahedron Letters (2001), 42(9), 1631-1633
SO
    CODEN: TELEAY; ISSN: 0040-4039
PΒ
     Elsevier Science Ltd.
DT
     Journal
LА
     English
CC
     26-4 (Biomolecules and Their Synthetic Analogs)
     CASREACT 134:366704
OS
    A stereocontrolled approach to substituted piperidones and piperidines is
AΒ
     presented, and their utility as intermediates for the synthesis of
     flavopiridol D-ring analogs is described.
     piperidine flavopiridol analog stereoselective prepn; piperidone
ST
     flavopiridol analog stereoselective prepn
TТ
     Stereoselective synthesis
        (of piperidones and piperidines as flavopiridol D-ring analogs)
     75-98-9
IT
     RL: RGT (Reagent); RACT (Reactant or reagent)
        (preparation of)
TΤ
     146426-40-6P, Flavopiridol
     RL: PNU (Preparation, unclassified); PREP (Preparation)
        (stereoselective preparation of piperidones and piperidines as flavopiridol
        D-ring analogs)
IT
     78-39-7
              610-96-8, Methyl 2-chlorobenzoate
                                                    830-79-5,
     2,4,6-Trimethoxybenzaldehyde 4202-14-6
                                               5927-18-4
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (stereoselective preparation of piperidones and piperidines as flavopiridol
        D-ring analogs)
TТ
     97024-78-7P
                   100257-91-8P
                                  115130-74-0P
                                                  340203-15-8P
                                                                 340203-16-9P
                                   340203-19-2P
     340203-17-0P
                    340203-18-1P
                                                  340203-20-5P
                                                                  340203-21-6P
     340203-22-7P
                                   340203-24-9P
                                                   340203-25-0P
                                                                  340203-26-1P
                    340203-23-8P
     340203-27-2P · 340203-28-3P
                                   340203-29-4P
                                                  340203-30-7P
                                                                  340203-31-8P
     340203-32-9P
                    340203-34-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
```

(Reactant or reagent) (stereoselective preparation of piperidones and piperidines as flavopiridol D-ring analogs) IT 340203-33-0P 340203-35-2P RL: SPN (Synthetic preparation); PREP (Preparation) (stereoselective preparation of piperidones and piperidines as flavopiridol D-ring analogs) THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT (1) Gonzalez, F; Org Synth 1986, V64, P175 HCAPLUS (2) Johnson, W; J Am Chem Soc 1970, V92, P741 HCAPLUS (3) Kattige, S; US 4900727 1990 HCAPLUS (4) Naik, R; US 5284856 1988 HCAPLUS (5) Naik, R; Tetrahedron 1988, V44, P2081 HCAPLUS (6) Sedlacek, H; Int J Oncol 1996, V9, P1143 HCAPLUS (7) Sielecki, T; J Med Chem 2000, V43, P1 HCAPLUS IT 340203-32-9P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (stereoselective preparation of piperidones and piperidines as flavopiridol D-ring analogs) 340203-32-9 HCAPLUS RN CN 4H-1-Benzopyran-4-one, 2-(2-chlorophenyl)-8-[(3R,4S,5R)-3-hydroxy-1,5dimethyl-4-piperidinyl]-5,7-dimethoxy-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 340203-33-0P 340203-35-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (stereoselective preparation of piperidones and piperidines as flavopiridol D-ring analogs)
RN 340203-33-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2-(2-chlorophenyl)-5,7-dihydroxy-8-[(3R,4S,5R)-3-hydroxy-1,5-dimethyl-4-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 340203-35-2 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2-(2-chlorophenyl)-5,7-dihydroxy-8-[(2R,3R,4S)-3-hydroxy-1,2-dimethyl-4-piperidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L63 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:554970 HCAPLUS

DN 133:278492

ED Entered STN: 13 Aug 2000

TI Biotransformation of a C-glycosylflavone, abrusin 2"-O- β -D-apioside, by human intestinal bacteria

AU Li, Yan; Meselhy, Meselhy R.; Wang, Li-Quan; Ma, Chao-Mei; Nakamura, Norio; Hattori, Masao

CS Institute of Natural Medicine, Toyama Medical and Pharmaceutical University, Toyama, 930-0194, Japan

SO Chemical & Pharmaceutical Bulletin (2000), 48(8), 1239-1241 CODEN: CPBTAL; ISSN: 0009-2363

PB Pharmaceutical Society of Japan

DT Journal

LA English

CC 10-2 (Microbial, Algal, and Fungal Biochemistry)

GI

After anaerobic incubation of abrusin 2"-O- β -D-apioside (I) with a AB human fecal suspension, five metabolites were isolated and identified as abrusin, 1-(2',6'-dihydroxy-3',4'-dimethoxyphenyl)-3-(4"hydroxyphenyl)propan-1-one, 5,6-dimethoxybenzene-1,3-diol, 3-(4'-hydroxyphenyl)propionic acid, and 3-phenylpropionic acid. However, Me ether derivs. of abrusin (4'-O-methylabrusin and 4'-O-, 5-O-dimethylabrusin) resisted degradation under the same conditions.

abrusin apioside biotransformation intestinal bacteria

Ι

IT Intestinal bacteria

(biotransformation of abrusin apioside by human intestinal bacteria)

3681-93-4, Vitexin 211568-62-6, Precatorin II

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(biotransformation by human intestinal bacteria)

IT 120727-04-0

> RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(biotransformation of abrusin apioside by human intestinal bacteria) 120727-02-8, Abrusin 299404-85-6

RL: BPR (Biological process); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); PROC (Process)

(biotransformation of abrusin apioside by human intestinal bacteria) 501-52-0, 3-Phenylpropionic acid 501-97-3, 3-(4'-Hydroxyphenyl)propionic 13077-75-3

RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)

(biotransformation of abrusin apioside by human intestinal bacteria) RE.CNT THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD 22

IT

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IT 120727-04-0
   RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
        (biotransformation of abrusin apioside by human intestinal bacteria)
RN 120727-04-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 8-(2-O-D-apio-β-D-furanosyl-β-D-glucopyranosyl)-5-hydroxy-2-(4-hydroxyphenyl)-6,7-dimethoxy- (9CI) (CA INDEX NAME)
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Absolute stereochemistry. Rotation (-).

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L63 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
     1998:409308 HCAPLUS
AN
DN
     129:173045
ED
     Entered STN: 04 Jul 1998
     Saponins and C-glycosyl flavones from the seeds of Abrus precatorius
TI
     Ma, Chao-Mei; Nakamura, Norio; Hattori, Masao
AU
CS
     Research Institute for Wakan-Yaku (Traditional Sino-Japanese Medicines),
     Toyama Medical and Pharmaceutical University, Toyama, 930-0194, Japan
     Chemical & Pharmaceutical Bulletin (1998), 46(6), 982-987
SO
     CODEN: CPBTAL; ISSN: 0009-2363
     Pharmaceutical Society of Japan
PB
DΤ
     Journal
     English
LΑ
     11-1 (Plant Biochemistry)
CC
     Section cross-reference(s): 33
     Two new saponins, 3-0-[\beta-D-glucuronopyranosyl-(1 \rightarrow
AΒ
     2)-\beta-D-glucopyranosyl]hederagenin (named abrus-saponin I) and
     3-0-[\beta-D-glucuronopyranosyl-(1 \rightarrow 2)-\beta-D-
     glucopyranosyl]oleanolic acid 28-β-D-glucopyranosyl ester
     (abrus-saponin II), and three new flavones, 6-C-\beta-D-glucopyranosyl-
     4',5-dihydroxy-7,8-dimethoxyflavone (precatorin I), 6-C-[β-D-
     apiofuranosyl-(1 \rightarrow 2)-\beta-D-glucopyranosyl]-4',5-dihydroxy-7,8-
     dimethoxyflavone (precatorin II), 6-C-[\beta-D-apiofuranosyl-(1 \rightarrow
     2)-β-D-glucopyranosyl]-4',5-dihydroxy-7-methoxyflavone (precatorin
     III), were isolated from the seeds of Abrus precatorius L. together with
     twelve known compds. including a naturally new saponin,
     3-O-[\beta-D-glucuronopyranosyl-(1 \rightarrow 2)-\beta-D-glucopyranosyl]oleanolic acid. Their structures were determined on the basis
     of chemical and spectroscopic methods. In addition, the unusual NMR spectral
     behavior of the flavone C-glycosides is also discussed.
ST
     abrussaponin saponin precatorin flavone Abrus
ΙT
     Glycosides
     Glycosides
     RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP
     (Properties); PUR (Purification or recovery); BIOL (Biological study);
     OCCU (Occurrence); PREP (Preparation)
```

```
(C-flavonoid oxo; from seeds of Abrus precatorius)
TТ
     New natural products
        (abrus-saponin I (saponin))
IT
     New natural products
        (abrus-saponin II (saponin))
TΤ
     Saponins
     RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP
     (Properties); PUR (Purification or recovery); BIOL (Biological study);
     OCCU (Occurrence); PREP (Preparation)
        (from seeds of Abrus precatorius)
TΤ
     Molecular structure, natural product
        (of abrus-saponin I (saponin))
     Molecular structure, natural product
TT
        (of abrus-saponin II (saponin))
     Molecular structure, natural product
TТ
        (of precatorin I (C-glycosyl flavone))
     Molecular structure, natural product
TT
        (of precatorin II (C-glycosyl flavone))
IT
     Molecular structure, natural product
        (of precatorin III (C-glycosyl flavone))
     New natural products
IT
        (precatorin I (C-glycosyl flavone))
     New natural products
IT
        (precatorin II (C-glycosyl flavone))
IT
     New natural products
        (precatorin III (C-glycosyl flavone))
IT
     Abrus precatorius
        (saponins and C-glycosyl flavones from seeds of Abrus precatorius)
IT
     487-58-1
                526-31-8, Abrine
                                   1447-88-7
                                                6601-62-3
                                                              115330-90-0,
                        117210-04-5, Kaikasaponin I 117230-29-2, Kaikasaponin
     Kaikasaponin III
                         120727-02-8, Abrusin 120727-04-0
     III methyl ester
     134859-87-3 158275-42-4
                                 163597-20-4, Phaseoside IV
     RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
     BIOL (Biological study); OCCU (Occurrence)
        (from seeds of Abrus precatorius)
TT
     120727-05-1P, Precatorin I 211568-32-0P, Abrus saponin I 211568-33-1P,
                       211568-62-6P, Precatorin II 211568-81-9P, Precatorin
     Abrus saponin II
     RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP
     (Properties); PUR (Purification or recovery); BIOL (Biological study);
     OCCU (Occurrence); PREP (Preparation)
        (from seeds of Abrus precatorius)
              THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT 16
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     120727-04-0
     RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
     BIOL (Biological study); OCCU (Occurrence)
         (from seeds of Abrus precatorius)
     120727-04-0 HCAPLUS
RN
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CN 4H-1-Benzopyran-4-one, 8-(2-O-D-apio-β-D-furanosyl-β-Dglucopyranosyl)-5-hydroxy-2-(4-hydroxyphenyl)-6,7-dimethoxy- (9CI) (CA
INDEX NAME)

Absolute stereochemistry. Rotation (-).

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L63 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
     1994:319424 HCAPLUS
AN
DN
     120:319424
ED
     Entered STN: 25 Jun 1994
     Flavonoid glycosides from Cotoneaster thymaefolia
TI
     Palme, Elisa; Bilia, Anna Rita; De Feo, Vincenzo; Morelli, Ivano
ΑU
CS
     Dip. Chim. Bioorg., Univ. Pisa, Pisa, 56126, Italy
     Phytochemistry (1994), 35(5), 1381-2
CODEN: PYTCAS; ISSN: 0031-9422
SO
DT
     Journal
LΑ
     English
CC
     11-1 (Plant Biochemistry)
     Section cross-reference(s): 26, 33
     A new C-glycoside, vitexin-2''-O-\alpha-D-arabinofuranoside, was isolated
AΒ
     from the leaves of Cotoneaster thymaefolia. Vitexin, vitexin-2''-O-
     rhamnoside, rutin, quercetin 3-rhamnoside, 5,7,2',5'-tetrahydroxyflavanone and its 7-glucoside were also identified. The structures of the compds.
     were determined by spectroscopic methods.
ST
     Cotoneaster flavonoid glycoside isolation
     Cotoneaster thymaefolia
IT
         (flavonoid glycosides from leaves of, structures of)
IT
     Glycosides
     RL: BOC (Biological occurrence); BIOL (Biological study); OCCU
      (Occurrence)
         (flavonoid, from leaves of Cotoneaster thymaefolia, structure of)
     153-18-4, Rutin 522-12-3, Quercetin 3-rhamnoside
                                                              74175-75-0
TТ
     146555-77-3
     RL: BOC (Biological occurrence); BIOL (Biological study); OCCU
      (Occurrence)
         (from leaves of Cotoneaster thymaefolia)
TT
     155346-48-8, Vitexin-2''-O-\alpha-D-arabinofuranoside
     RL: BOC (Biological occurrence); PRP (Properties); BIOL (Biological
     study); OCCU (Occurrence)
         (structure and isolation of, from leaves of Cotoneaster thymaefolia)
     155346-48-8, Vitexin-2''-O-\alpha-D-arabinofuranoside
     RL: BOC (Biological occurrence); PRP (Properties); BIOL (Biological
     study); OCCU (Occurrence)
         (structure and isolation of, from leaves of Cotoneaster thymaefolia)
     155346-48-8 HCAPLUS
RN
     4H-1-Benzopyran-4-one, 8-(2-0-\alpha-D-arabinofuranosyl-\beta-D-
CN
     glucopyranosyl)-5,7-dihydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)
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L63 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:489078 HCAPLUS

DN 115:89078

ED Entered STN: 06 Sep 1991

TI Studies on leguminous plants. Part XIX. A new sapogenol and other constituents in abri semen, the seeds of Abrus precatorius L. I

AU Kinjo, Junei; Matsumoto, Kumiko; Inoue, Mutsumi; Takeshita, Takashi; Nohara, Toshihiro

CS Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, 862, Japan

SO Chemical & Pharmaceutical Bulletin (1991), 39(1), 116-19 CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

CC 11-1 (Plant Biochemistry)

Section cross-reference(s): 30, 63

GΙ

AB A new sapogenol, abrisapogenol J (I), was isolated from the methanolyzate of A. precatorius seeds, together with sophoradiol, its 22-0-acetate (II) and hederagenin Me ester. The structure of I was 3β,22β-dihydroxy-11-oxoolean-13(18)-ene based on hetero nuclear multiple bonds correlation (HMBC) spectroscopy. In addition, various compds., tri-Me tryptophan dipolar ion (III) kaikasaponin III Me ester, abrine, abrusin and its 2''-0-apioside were obtained from the methanolic extract. This is the first example of the isolation of compds. I-III in nature.

ST oleanene triterpene Abrus seed; Abrus seed compn; triterpene Abrus seed; abrisapogenol J Abrus seed; sapogenol Abrus seed; sophoradiol acetate Abrus seed; tryptophan trimethyl Abrus seed

IT Nomenclature, new natural products

(abrisapogenol J (triterpene))

(of abrisapogenol J (triterper

IT Triterpenes and Triterpenoids

RL: BIOL (Biological study)

(oleanene, from Abrus precatorius seeds, isolation and structure of) IT Abrus precatorius (sapogenol and other constituents of seeds of, isolation and structure of) 526-31-8, Abrine 6822-47-5, Sophoradiol IT 487-58-1 17736-04-8, Hederagenin methyl ester 117230-29-2, Kaikasaponin III methyl ester 120727-02-8, Abrusin 120727-04-0 RL: BIOL (Biological study) (from Abrus precatorius seeds) IT 86425-27-6, Sophoradiol 22-0-acetate 135308-91-7, Abrisapogenol J RL: BIOL (Biological study) (from Abrus precatorius seeds, isolation and structure of) 120727-04-0 IT RL: BIOL (Biological study) (from Abrus precatorius seeds) RN 120727-04-0 HCAPLUS 4H-1-Benzopyran-4-one, 8-(2-O-D-apio- β -D-furanosyl- β -Dglucopyranosyl)-5-hydroxy-2-(4-hydroxyphenyl)-6,7-dimethoxy- (9CI) (CA

Absolute stereochemistry. Rotation (-).

INDEX NAME)

L63 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN AN 1989:439717 HCAPLUS DN 111:39717 Entered STN: 05 Aug 1989 ED TI Convenient synthesis of $C-\beta-D$ -glucopyranosyl arenes. Synthesis of 5,7,4'-tri-0-methylvitexin Frick, Wendelin; Schmidt, Richard R. ΑU CS Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger. SO Liebigs Annalen der Chemie (1989), (6), 565-70 CODEN: LACHDL; ISSN: 0170-2041 DTJournal LА German CC 33-3 (Carbohydrates) os CASREACT 111:39717 GI

III

MeO

IT

119529-73-6P

119529-74-7P

AΒ Reaction of 4,2,6-MeO(R2)C6H2Li (R = H, OMe) and flavanones I with the D-glucoses II (R = CH2Ph, CH2OMe) furnished the C-glucosyl derivs. in good yields. Hydrogenolytic debenzylation in the presence of AcOH leads directly to the thermodynamically stable $C-(\beta-D-glucopyranosyl)$ arenes. 5,7,4'-Tri-O-methylvitexin (III) is obtained in two steps from the flavonoid glycoside. STglucopyranosyl arene; arene glucoside; vitexin trimethyl ether IT Glycosides RL: SPN (Synthetic preparation); PREP (Preparation) (C-, glucopyranosylarenes, preparation of) IT 66074-95-1 119529-70-3 RL: PROC (Process) (acetalization of) TT 53929-48-9 RL: RCT (Reactant); RACT (Reactant or reagent) (methoxymethylation of) IT 119529-65-6P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and acetalhydrolysis of) 119529-60-1P IT 119529-59-8P 119529-61-2P 86762-94-9P 119529-62-3P 119529-63-4P 119529-64-5P 119529-71-4P 119529-72-5P 119529-75-8P 119529-76-9P 119529-81-6P 119529-82-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and acetylation of) IT 157495-58-4P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and bromination of) ΙT 119529-67-8P 119529-80-5P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and cyclization of) 119529-58-7P 119592-94-8P 119677-12-2P 119677-13-3P IT 119529-57-6P 119677-14-4P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and hydrogenolysis of)

119529-78-1P

119529-83-8P

119529-77-0P

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119567-06-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and oxidation of)
IT
     157495-49-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, with glucose derivative)
     119529-66-7P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, with lithioarenes)
                                   20197-48-2P
                                                  38714-70-4P
     9002-23-7P, Amberlite IR-120
                                                                 119529-55-4P
IT
     119529-56-5P 119529-79-2P 119529-84-9P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
IT
     93414-73-4P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation, hydrogenolysis, and acetylation of)
IT
     34425-71-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with glucose derivative)
IT
     14774-77-7
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with glucose derivs.)
IT
     78699-85-1
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with lithioarenes)
IT
     119529-79-2P 119529-84-9P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN
     119529-79-2 HCAPLUS
     4H-1-Benzopyran-4-one, 5,7-dimethoxy-2-(4-methoxyphenyl)-8-(2,3,5,6-tetra-
CN
     O-acetyl-α-D-glucofuranosyl) - (9CI) (CA INDEX NAME)
```

Absolute stereochemistry.

RN 119529-84-9 HCAPLUS

CN 4H-1-Benzopyran-4-one, 5,7-dimethoxy-2-(4-methoxyphenyl)-8-(2,3,5,6-tetra-O-acetyl-β-D-glucofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
L63
     1989:228586 HCAPLUS
AN
DN
     110:228586
ED
     Entered STN: 25 Jun 1989
TI
     8-C-Glucosylscutellarein 6,7-dimethyl ether and its 2"-O-apioside from
     Abrus precatorius
ΑU
     Markham, Kenneth R.; Wallace, James W.; Babu, Y. Niranjan; Murty, V.
     Krishna; Rao, M. Gopala
CS
     Chem. Div., DSIR, Petone, N. Z.
     Phytochemistry (1988), Volume Date 1989, 28(1), 299-301 CODEN: PYTCAS; ISSN: 0031-9422
SO
DT
     Journal
T.A
     English
CC
     11-1 (Plant Biochemistry)
     Section cross-reference(s): 26, 33
GΙ
```

8-C-Glucosylscutellarein 6,7-dimethyl ether (abrusin, I) and its AB 2''-O-apioside were identified as minor components in the seeds of A. precatorius. Their structures were determined by UV-visible and 1H- and 13C-NMR spectrometry and chemical methods. Both are new natural products and are the first examples of flavone-C-glycosides containing a trioxygenated A-ring. Abrusin 2''-O-apioside is the only known apioside of a flavone-C-glycoside. Abrus seed abrusin apioside; abrusin apioside flavone glycoside Abrus ST

IT Nomenclature, new natural products

(abrusin (flavonoid glycoside))

Ι

IT Abrus precatorius

(abrusin and abrusin apioside from seeds of, isolation and structure

```
of)
TT
     Molecular structure, natural product
        (of abrusin (flavonoid glycoside))
IT
     Glycosides
     RL: BIOL (Biological study)
        (flavone C-, from Abrus precatorius, isolation and structure of
        abrusin)
IT
     120727-02-8, Abrusin 120727-04-0
     RL: BIOL (Biological study)
        (from Abrus precatorius seeds, isolation and structure of)
IT
     120727-05-1P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
IT
     120727-04-0
     RL: BIOL (Biological study)
        (from Abrus precatorius seeds, isolation and structure of)
RN
     120727-04-0 HCAPLUS
CN
     4H-1-Benzopyran-4-one, 8-(2-O-D-apio-\beta-D-furanosyl-\beta-D-
```

glucopyranosyl)-5-hydroxy-2-(4-hydroxyphenyl)-6,7-dimethoxy- (9CI) (CA

Absolute stereochemistry. Rotation (-).

INDEX NAME)

L63 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN 1987:575780 HCAPLUS ANDN 107:175780 ED Entered STN: 14 Nov 1987 TI Preparation of pyridinylflavone derivatives as calcium antagonists and smooth muscle relaxants IN Leonardi, Amedeo; Pennini, Renzo; Cazzulani, Pietro; Nardi, Dante PΑ Recordati S. A. Chemical and Pharmaceutical Co., Switz. SO Eur. Pat. Appl., 32 pp. CODEN: EPXXDW DT Patent English LA IC ICM C07D405-04 ICS C07D405-14; A61K031-445 CC 26-4 (Biomolecules and Their Synthetic Analogs) Section cross-reference(s): 1, 27 FAN.CNT 1 PATENT NO. KIND APPLICATION NO. DATE DATE ----- ----_____ EP 1986-830300 PT EP 223744 19870527 19861020 A2 EP 223744 АЗ 19880914 EP 223744 B1 19920311 R: AT, BE, CH, DE, ES, FR, GB, GR, LI, LU, NL, SE IL 80229 **A1** 19901105 IL 1986-80229 19861003 NO 1986-4108 NO 8604108 19870423 19861015 Α

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FI	8604260		A	19870423	FΙ	1986-4260	19861021
FI	89167		В	19930514			
FI	89167		C	19930825			
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JP	07072186		B4	19950802			
HU	45525		A2	19880728	HU	1986-4363	19861021
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CA	1330994		A1	19940726	CA	1986-520953	19861021
DK	8605063		A	19870423	DK	1986-5063	19861022
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AU	596382		B2	19900503			
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US	4806534		Α	19890221	US	1986-921397	19861022
PRAI IT	1985-225	78	A	19851022			
EP	1986-830	300	A	19861020			
CLASS							
PATENT	NO.	CLASS	PATENT	FAMILY CLASS	IFI	CATION CODES	
EP 2237	744	ICM	C07D405				
		ICS		-14; A61K031			
US 4806	5534	NCL				00; 514/253.110;	
						00; 544/131.000;	
						00; 546/269.700;	
						00; 546/274.700;	546/275.400;
			546/279	.100; 546/28	3.10	00	
GI							

$$\begin{array}{c|c} & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

AB Title compds. I (R, R1 = C1-4 alkyl, formylalkyl, cyanoalkyl, C1-4 hydroxyalkyl; R2, R3 = C1-6 alkyl, C2-6 alkenyl, -alkynyl, C5-7 cycloalkyl, aralkyl, Ph, etc., R4R5N-alkyl; R4, R5 = H, alkyl, Ph, etc., or R4R5N = heterocyclyl) their optical isomers, diastereomers, and salts were prepared as calcium antagonists and smooth muscle relaxants.

3-Methyl-8-formylflavone, MeCOCH2CO2Me, MeC(NH2):CHCO2Me and EtOH were refluxed to give I (R-R3 = Me) (II). II had IC50 of 5.55 x 10-9 nM on Ca-antagonistic binding sites using rat brain membranes. in vitro. The activity on urodynamic parameters was detected by cystometric recordings on rats given II at 10 mg/kg orally; the changes in bladder volume capacity and micturition pressure were +18 and -14%, resp.

flavonylpyridinedicarboxylate prepn drug; calcium antagonist flavonylpyridinedicarboxylate prepn; muscle smooth relaxant flavonylpyridinedicarboxylate prepn

IT Bladder

(muscle relaxants for, methylflavonyldihydropyridinedicarboxylates as)

```
IT
    Muscle relaxants
        (smooth, methylflavonyldihydropyridinedicarboxylates)
IT
     7440-70-2, biological studies
    RL: BIOL (Biological study)
        (antagonists for, flavone derivs. as)
IT
     5470-11-1, Hydroxylamine hydrochloride
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (condensation of, with formyldihydropyridinedicarboxylate, cyano derivative
TT
    54527-68-3, \beta-Chloroethyl acetoacetate 60705-25-1, Methyl
     4,4-dimethoxyacetoacetate
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (condensation of, with methylformylflavone)
IT
     43107-08-0, 2-Cyanoethyl 3-aminocrotonate
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of with chloroethyl (methylflavonmethylidine)acetoac
        etate)
IT
     14205-46-0, Isopropyl 3-aminocrotonate
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of with chloroethyl (methylflavonyl)acetoacetate)
IT
     14205-39-1, Methyl 3-aminocrotonate
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with Me acetoacetate and methylformylflavone)
TT
     105-45-3, Methyl acetoacetate
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with Me aminocrotonate and methylformylflavone)
TΤ
     110714-57-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with cyanoethyl aminocrotonate)
IT
     110714-51-7
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with methylformylflavone and piperidinoethyl
        acetoacetate)
IT
    108852-41-1
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with methylformylflavone and piperidoethyl
        aminocrotonate)
IT
     103085-54-7P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation and condensation of, with acetoacetate)
IT
     110714-88-0P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and cyclocondensation of, with Me aminocrotonate)
ΙT
    110714-52-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and cyclocondensation of, with iso-Pr aminocrotonate)
IT
     110714-59-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and esterification of)
TT
    110714-89-1P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and hydrolysis of)
                   110714-50-6P
                                   110714-53-9P
                                                  110714-54-0P
                                                                  110714-55-1P
     110714-49-3P
                                                  110714-61-9P
    110714-56-2P
                    110714-58-4P
                                   110714-60-8P
                                                                 110714-62-0P
    110714-63-1P
                  110714-64-2P
                                   110714-65-3P
                                                  110714-66-4P
                                                                 110714-67-5P
     110714-68-6P
                  110714-69-7P
                                   110714-70-0P
                                                  110714-71-1P
                                                                 110714-72-2P
                                                                 110714-77-7P
                                   110714-75-5P
                                                  110714-76-6P
     110714-73-3P
                  110714-74-4P
     110714-78-8P 110714-79-9P 110714-80-2P 110714-81-3P
                                   110714-84-6P
                                                  110714-85-7P
     110714-82-4P
                    110714-83-5P
                                                                  110714-86-8P
    110714-87-9P
                    110714-90-4P
                                   110714-91-5P
                                                  110714-92-6P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of, as calcium antagonist and smooth muscle relaxant)
```

RL: RCT (Reactant); RACT (Reactant or reagent) (reduction of, formyl analog from)

IT 110714-79-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as calcium antagonist and smooth muscle relaxant)

RN 110714-79-9 HCAPLUS

CN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(3-methyl-4-oxo-2-phenyl-4H-1-benzopyran-8-yl)-, 2-(1H-imidazol-1-yl)ethyl methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{H} & \text{Me} \\ \hline & \text{N} & \text{O} \\ \hline & \text{C} & \text{O} & \text{CH}_2 - \text{CH}_2 \\ \hline & \text{N} \\ \hline & \text{O} \\ \hline & \text{Me} \\ \hline & \text{Me} \\ \end{array}$$

L63 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1985:62091 HCAPLUS

DN 102:62091

ED Entered STN: 24 Feb 1985

TI Chromone- and thiochromone-substituted 1,4-dihydropyridine derivatives and their use in pharmaceuticals

IN Goldmann, Siegfried; Franckowiak, Gerhard; Schramm, Matthias; Thomas, Guenter; Gross, Rainer

PA Bayer A.-G., Fed. Rep. Ger.

SO Ger. Offen., 42 pp.

CODEN: GWXXBX

DT Patent

LA German

IC C07D405-04; C07D405-14; C07D413-12; C07D413-14; C07D417-04; C07D417-06; C07D417-14; C07D409-10; A61K031-44

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 1

FAN.CNT 2

L'MIA'	CIAT	4													
	PAT	TENT	NO.			KINI)	DATE		1	API	PLICATION	NO.	DATE	
PI	DE	3311	005			A1		1984	0927	1	DE	1983-331	L005	198303	25
	DK	8401	453			Α		1984	0926	1	DK	1984-1453	3	198402	29
	DK	1637	33			В		1992	0330						
	NO	8400	951			A		1984	0926	1	NO	1984-951		198403	13
	US	4540	789			A		1985	0910	1	US	1984-5894	136	198403	14
	ΕP	1231	12			A2		1984	1031	1	ΕP	1984-1029	903	198403	16
	ΕP	1231	12			A3		1987	0722						
	ΕP	1231	12			B1		1988	0921						
		R:	AT,	BE,	CH,	DE,	FR,	GB,	IT,	LI,	LU	J, NL, SE			
	ΑT	3736	7			E		1988	1015	7	ΑT	1984-1029	903	198403	16
	ΑU	8425	914			A1		1984	0927	2	UΑ	1984-2591	L4	198403	20
	ΑU	5580	35			B2		1987	0115						
	ES	5308	02			A1		1984	1101	1	ES	1984-5308	302	198403	21
	FΙ	8401	154			A		1984	0926	1	FI	1984-1154	1	198403	22
	FI	8246	3			В		1990	1130						
	FI	8246	3			C		1991	0311						

	JP	59176281		A2	1984	1005	JP	198	4-54581		19	840323
	JР	05049671		B4	19930	0726						
	ZA	8402165		A	1984:	1031	ZA	198	4-2165		19	840323
	HU	34186		0	19850	0228	HU	198	4-1178		19	840323
	HU	191302		В	19870	0227						
	CA	1236460		A1	19880	0510	CA	198	4-450362	2	19	840323
	US	4628107		A	1986	1209	US	198	5-750573	L	19	850628
	ES	552230		A1	19870	0501	ES	198	6-552230)	19	860220
	ES	552231		A1	19870	0501	ES	198	6-552233	L	19	860220
	ES	552232		A1	19870	0501	ES	198	6-552232	3	19	860220
PRAI	DE	1983-3313	1004	Α	19830	0325						
	DE	1983-3313	1005	A	19830	0325						
	US	1984-5894	136	A2	19840	0314						
	US	1984-589	515	A2	19840	0314						
	EΡ	1984-1029	903	A	19840	0316						
CLAS	S											
PAT	ENT	NO.	CLASS	PATENT 1	FAMIL:	Y CLAS	SSIFIC	CATI	ON CODES	3		
										· ·	. .	
DE .	3311	.005	IC	C07D405								
				C07D413								C
		=		C07D417					OIC			
US ·	4540	789	NCL	514/337								
				544/364								
				546/167								
				546/270								
				546/274								
				546/276								
				546/280		546/2	280.40	JO;	546/281	400;	546/28	3.100;
		4.05	NOT.	546/283		- 4 - 1 -			/		540/55	
US ·	4628	107	NCL	549/023								
									549/402			

$$R_n$$
 X
 ZR^1
 R^2Z^1CO
 R^3
 R^4
 R^5

Ι

GΙ

Antihypotensive and cardiotonic (no data) title compds. [I; R = halo; R1 = H, (un) substituted alkyl, aryl, heteroaryl; R2 = (un) substituted alkyl, alkenyl, cycloalkyl, aryl, heteroaryl; R3, R5 = H, (un) substituted alkyl, alkenyl, cycloalkyl, optionally with heteroatom interrupters; R4 = H, (un) substituted alkyl; R6 = H, alkyl, polyfluoroalkyl, CO2H, NO2, cyano, halo; Z = bond, alkylene, oxaalkylene, thiaalkylene; Z1 = bond, O, S, R7N; R7 = H, alkyl; n = 0-3] were prepared Thus, 2-phenyl-4-oxo-4H-2-benzopyran-8-carboxaldehyde, H2NCMe:CHCO2Me, and MeCOCH2NO2 were refluxed 3 h in EtOH to give I (R1 = Ph, R2 = R3 = R5 = Me, R4 = H, R6 = NO2, X = Z1 = O; Z = bond, n = 0).

ST cardiotonic benzopyranylpyridinecarboxylate; antihypotensive benzopyranylpyridinecarboxylate; benzopyrancarboxaldehyde cyclocondensation aminocrotonate nitroacetone; pyridinecarboxylate benzopyranyl benzothiopyranyl

IT Antihypotensives

```
(benzopyranyl- and benzothiopyranylpyridinecarboxylates)
TΤ
     Cyclocondensation reaction
        (of aminocrotonates, nitroacetone, and benzopyran- and
        benzothiopyrancarboxaldehydes)
IT
        (stimulants, benzopyranyl- and benzothiopyranylpyridinecarboxylates)
IT
     1118-61-2
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with acetoacetates and benzopyran- and
        benzothiopyrancarboxaldehydes)
IT
     591-60-6
               10230-68-9
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with aminocrotonates and benzopyran- and
        benzothiopyrancarboxaldehydes)
IT
     87626-84-4
                  94127-35-2
                               94127-37-4
                                             94127-38-5
                                                          94127-39-6
     94127-71-6
                  94127-72-7
                               94419-93-9
                                             94419-94-0
                                                          94420-02-7
     94420-03-8
                  94420-04-9
                               94420-05-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with aminocrotonates and nitroacetone)
IT
     14205-39-1
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with nitroacetone and benzopyran- and
        benzothiopyrancarboxaldehydes)
IT
                                 94419-97-3P
     94419-95-1P
                   94419-96-2P
                                                94419-98-4P
                                                              94419-99-5P
     94420-00-5P
                   94420-01-6P
                                 94420-06-1P
                                                94420-07-2P
                                                              94420-08-3P
     94420-09-4P
                   94420-10-7P
                                 94420-11-8P
                                                94420-12-9P 94420-13-0P
     94420-14-1P
                   94420-15-2P
                                 94420-16-3P
                                                94420-17-4P
     94420-18-5P
                   94420-19-6P
                                 94420-20-9P
                                                94420-21-0P
                                                              94420-22-1P
     94420-23-2P
                   94420-24-3P
                                 94420-25-4P
                                                94420-28-7P
                                                              94420-29-8P
     94420-30-1P
                   94420-31-2P
                                 94420-32-3P
                                                94420-33-4P
                                                              94420-34-5P
     94420-35-6P
                   94420-36-7P
                                 94420-37-8P
                                                94420-38-9P
                                                              94426-33-2P
     94444-51-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
IT
     94420-13-0P 94420-14-1P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN
     94420-13-0 HCAPLUS
CN
     3-Pyridinecarboxylic acid, 1,4-dihydro-2,6-dimethyl-5-nitro-4-[4-oxo-2-(3-
     thienyl)-4H-1-benzopyran-8-yl]-, ethyl ester (9CI) (CA INDEX NAME)
               Me
   Мe
```

RN 94420-14-1 HCAPLUS
CN 3-Pyridinecarboxylic acid, 1,4-dihydro-2,6-dimethyl-5-nitro-4-[4-oxo-2-(3-thienyl)-4H-1-benzopyran-8-yl]-, butyl ester (9CI) (CA INDEX NAME)

L63 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1985:45915 HCAPLUS

DN 102:45915

Entered STN: 09 Feb 1985 ED

Chromone- and thiochromone-substituted 1,4-dihydropyridine lactones and ΤI their use in pharmaceuticals

IN Goldmann, Siegfried; Bossert, Friedrich; Schramm, Matthias; Thomas, Guenter; Gross, Rainer

Bayer A.-G. , Fed. Rep. Ger. Ger. Offen., 15 pp. PA

so

CODEN: GWXXBX

DT Patent

LΑ German

C07D491-048; A61K031-44; A61K031-435 IC

CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

FAN.CNT 1

FAIN.	CNI I	WT.170	D3.000	A D D T T CA TO T A VO	D. 1. C.
	PATENT NO.			APPLICATION NO.	
ΡI	DE 3311003		19840927		19830325
PI	DE 3311003	ΑT	19840927		
	DK 8401449	A B C	19840926	DK 1984-1449	19040229
	DK 158950	В	19900806		
	DK 158950	7.0	19901231	DD 1004 100650	10040010
	EP 123095			EP 1984-102659	19840312
	EP 123095				
	EP 123095		19881026		
	R: AT, BE, CH	, DE, FR	, GB, IT,	LI, LU, NL, SE	
	AT 38229 NO 8400950	E	19881115	AT 1984-102659	
	NO 8400950	A	19840926	NO 1984-950	19840313
	NO 160659 NO 160659	В	19890206		
	US 4555512	Α		US 1984-589614	
	ES 530800	A1		ES 1984-530800	19840321
	FI 8401153	A1 A	19840926	FI 1984-1153	19840322
	FI 81100	В	19900531		
	FI 81100				
	IL 71314			IL 1984-71314	
	ZA 8402166	Α	19841031		19840323
	HU 33808	0	19841228	HU 1984-1175	19840323
	HU 189849	B A1	19860828		
	CA 1211109	A1	19860909	CA 1984-450361	19840323
	JP 59193887	A2	19841102	JP 1984-57202	19840324
	JP 03016955	B4	19910306		
	AU 8426099	A1	19840927	AU 1984-26099	19840326
	AU 564838	B2	19870827		
	ES 552277	A1	19870901	ES 1986-552277	19860221
	ES 552278	A1	19870901	ES 1986-552278	19860221
	ES 552279	A1	19870901	ES 1986-552279	19860221
	ES 552280	A1	19870901	ES 1986-552280	19860221
PRAI	DE 1983-3311003	Α	19830325		
	EP 1984-102659	Α	19840312		

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CLASS
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PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

DE 3311003 IC C07D491-048IC A61K031-44IC A61K031-435
US 4555512 NCL 514/302.000; 514/232.500; 514/233.800; 514/234.500;
544/127.000; 546/115.000
OS CASREACT 102:45915
GI
```

$$R_n$$
 X
 ZR^1
 R^4Z^1CO
 R^3
 R^2

Cardiotonic and hypoglycemic (no data) title compds. [I; R = H, halo; R1 = aliphatic, alkoxycarbonyl, (un) substituted aromatic, heteroarom.; R2 = H, (un) substituted alkyl; R3 = H, (un) substituted alkyl, alkenyl, cycloalkyl, cycloalkenyl, optionally interrupted by O, S, SO2, R5N; R4 = (un) substituted straight- or branched-chain or cyclic hydrocarbon; R5 = H, alkyl; Z = bond, alkylene, alkenylene, optionally interrupted by O, S; Z1 = bond, O, S, R5N; n = 0-3] were prepared Thus, 4-oxo-2-phenyl-4H-thiochromene-8-carboxaldehyde was refluxed in EtOH with H2NCMe:CHCO2Et and ClCH2COCH2CO2Me to give I (R1 = Ph, R2 = H, R3 = Me, R4 = Et, Z = bond, Z1 = O, n = 0).

ST furopyridinecarboxylate benzopyranyl benzothiopyranyl; benzopyranone furopyridinyl; benzothiopyranone furopyridinyl; benzothiopyrancarboxaldehyde cyclocondensation acetoacetate aminocrotonate; cardiotonic furopyridinecarboxylate; hypoglycemic furopyridinecarboxylate

IT Heart

(contraction of, furopyridinecarboxylates effect on)

IT Antidiabetics and Hypoglycemics

(furopyridinecarboxylates)

Ι

IT Cyclocondensation reaction

(of acetoacetates with aminocrotonates and benzopyrancarboxaldehydes)

IT 87626-84-4 94127-29-4 94127-30-7 94127-34-1 94127-35-2 94127-36-3 94127-37-4 94127-38-5 94127-39-6 94127-71-6 94127-72-7 94127-74-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(cyclocondensation of, with acetylacetates and aminocrotonates)

IT 141-97-9 7318-00-5 14205-39-1 14205-41-5 14205-43-7 14205-46-0 24057-46-3 27618-18-4 39562-76-0 43107-11-5 50899-10-0 52937-87-8 53055-18-8 61312-61-6 77075-95-7 94127-31-8

94127-32-9 94127-33-0

RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclocondensation of, with acetylacetates and
 benzopyrancarboxaldehydes)

IT 32807-28-6

RL: RCT (Reactant); RACT (Reactant or reagent) (cyclocondensation of, with aminocrotonate and benzopyrancarboxaldehyde derivative)

IT 35594-15-1

RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclocondensation of, with aminocrotonates and
 benzopyrancarboxaldehydes)

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IT
     94127-73-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and cyclocondensation of, with acetylacetates and
        benzopyrancarboxaldehydes)
IT
     92089-08-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and cyclocondensation of, with aminocrotonate)
TΤ
     94127-42-1P
                  94127-43-2P
                                 94127-44-3P
                                                94127-45-4P
                                                              94127-46-5P
     94127-47-6P
                   94127-48-7P
                                 94127-49-8P
                                                94127-50-1P
                                                              94127-51-2P
     94127-52-3P
                   94127-53-4P
                                 94127-54-5P
                                                94127-55-6P
                                                              94127-56-7P
     94127-57-8P
                   94127-58-9P
                                 94127-59-0P
                                                              94127-61-4P
                                                94127-60-3P
     94127-62-5P
                   94127-63-6P
                                 94127-64-7P
                                                94127-65-8P
                                                              94127-66-9P
     94127-67-0P
                   94127-68-1P
                                 94127-69-2P 94127-70-5P
     94152-44-0P
                   96300-87-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
TΤ
     94127-70-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
     94127-70-5 HCAPLUS
RN
     Furo [3,4-b] pyridine-3-carboxylic acid, 1,4,5,7-tetrahydro-2-methyl-5-oxo-4-
     [4-oxo-2-(3-thienyl)-4H-1-benzopyran-8-yl]-, ethyl ester (9CI) (CA INDEX
     NAME)
```

GΙ

```
L63 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
     1984:68617 HCAPLUS
AN
     100:68617
DN
     Entered STN: 12 May 1984
ED
     Sugar ring isomerization in C-arabinosylflavones
тT
ΑU
     Besson, Elisabeth; Chopin, Jean
     Lab. Chim. Biol., Univ. Claude Bernard Lyon I, Villeurbanne, 69622, Fr.
CS
     Phytochemistry (Elsevier) (1983), 22(9), 2051-6 CODEN: PYTCAS; ISSN: 0031-9422
SO
DT
     Journal
     English
LΑ
     33-3 (Carbohydrates)
CC
     Section cross-reference(s): 26
```

Τ

```
Acid isomerization of 6-C-\alpha-L-arabinopyranosylacacetin, prepared by
     condensation reaction of acacetin with β-bromo-2,3,4-tri-O-acetyl-L-
     arabinopyranose, at 100° for 45 min gave the glycoacacetins I (R =
     \beta-L-arabinopyranosyl, \beta-L-arabinofuranosyl; R1 = R2 = H, R3 =
     Me) without any Wessely-Moser isomerization. Similar treatment of
     molludistin (I; R = R3 = H, R1 = \alpha-L-arabinopyranosyl, R2 = Me) (II)
     gave a mixture of II and I (R = R3 = H, R1 = \alpha-L-arabinopyranosyl, R2
     = Me). This is the 1st report of sugar ring isomerization in
     C-glycosylflavones. The pyranosyl and furanosyl isomers were easily separated
     after permethylation.
ST
     isomerization molludistin arabinopyranosylacacetin; acacetin
     arabinopyranosyl isomerization; flavone arabinosyl isomerization;
     arabinosylflavone isomerization
TТ
     Isomerization
        (of sugar ring of arabinosylflavones)
     480-44-4
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (arabinofuranosylation and arabinopyranosylation of)
IT
                  50730-31-9
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (condensation reaction of, with acacetin)
TТ
     66274-25-7
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (isomerization of)
IT
     88718-27-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and isomerization of)
                  88718-25-6P
                                 88718-26-7P
                                                88718-28-9P
                                                               88718-29-0P
IT
     88718-24-5P
                   88729-53-7P
     88718-30-3P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
IT
     88718-30-3P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN
     88718-30-3 HCAPLUS
     4H-1-Benzopyran-4-one, 8-α-L-arabinofuranosyl-5-hydroxy-2-(4-
CN
     hydroxyphenyl) - 7-methoxy- (9CI) (CA INDEX NAME)
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=> b uspatall
FILE 'USPATFULL' ENTERED AT 16:02:11 ON 13 OCT 2005
CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)
FILE 'USPAT2' ENTERED AT 16:02:11 ON 13 OCT 2005
CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)
=> d bib abs fhitstr hitrn 166 1
L66 ANSWER 1 OF 3 USPATFULL on STN
       2004:139405 USPATFULL
ΔN
ΤI
       Inhibitors of cyclin-dependent kinases and their use
IN
       Lal, Bansi, Mumbai, INDIA
       Joshi, Kalpana, Thane, INDIA
       Kulkarni, Sanjeev, Mumbai, INDIA
       Mascarenhas, Malcolm, Mumbai, INDIA
       Kamble, Shrikant, Mumbai, INDIA
       Rathos, Maggie Joyce, Thane, INDIA
       Joshi, Rajendrakumar, Mumbai, INDIA
PΤ
       US 2004106581
                               20040603
                          A1
                               20030701 (10)
       US 2003-611539
ΑI
                          A1
       IN 2002-6162002
                           20020708
PRAI
       US 2002-397326P
                           20020719 (60)
DT
       Utility
       APPLICATION
FS
       FROMMER LAWRENCE & HAUG LLP, 745 Fifth Avenue, New York, NY, 10151
LREP
CLMN
       Number of Claims: 23
       Exemplary Claim: 1
ECL
       6 Drawing Page(s)
DRWN
LN.CNT 5448
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
       The present invention relates to novel compounds for the inhibition of
       cyclin-dependent kinases, and more particularly, to chromenone
       derivatives of formula (Ia),
                                      ##STR1##
```

wherein R.sub.1, R.sub.2, R.sub.3, R.sub.4, R.sub.5, R.sub.6, R.sub.7 and A have the meanings indicated in the claims. The invention also relates to processes for the preparation of the compounds of formula (Ia), to methods of inhibiting cyclin-dependent kinases and of inhibiting cell proliferation, to the use of the compounds of formula (Ia) in the treatment and prophylaxis of diseases, which can be treated or prevented by the inhibition of cyclin-dependent kinases such as cancer, to the use of the compounds of formula (Ia) in the preparation of medicaments to be applied in such diseases. The invention further relates to compositions containing a compound of formula (Ia) either alone or in combination with another active agent, in admixture or otherwise in association with an inert carrier, in particular

pharmaceutical compositions containing a compound of formula (Ia) either alone or in combination with another active agent, together with pharmaceutically acceptable carrier substances and auxiliary substances.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 647019-53-2P

(preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent kinases)

RN 647019-53-2 USPATFULL

CN 4H-1-Benzopyran-4-one, 2-(2-chlorophenyl)-8-[(2R,3S)-2-(hydroxymethyl)-1-methyl-3-pyrrolidinyl]-5,7-dimethoxy-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

```
IT
    647019-53-2P 647019-54-3P 647019-55-4P
     647019-56-5P 647019-57-6P 647019-58-7P
     647019-59-8P 647019-60-1P 647019-61-2P
     647019-62-3P 647019-63-4P 647019-64-5P
      647019-65-6P 647019-66-7P 647019-67-8P
     647019-68-9P 647019-69-0P 647019-70-3P
     647019-71-4P 647019-72-5P 647019-73-6P
     647019-74-7P 647019-75-8P 647019-76-9P
     647019-77-0P 647019-78-1P 647019-79-2P
     647019-81-6P 647019-82-7P 647019-84-9P
      647019-85-0P 647019-86-1P 647019-87-2P
     647019-88-3P 647019-89-4P 647019-90-7P
     647019-91-8P 647019-92-9P 647019-93-0P
     647019-94-1P 647019-95-2P 647019-96-3P
     647019-97-4P 647019-98-5P 647019-99-6P
      647020-00-6P 647020-01-7P 647020-02-8P
      647020-03-9P 647020-04-0P 647020-05-1P
     647020-06-2P 647020-07-3P 647020-08-4P
      647020-09-5P 647020-19-7P 647020-20-0P
      647020-21-1P 647020-22-2P 647020-23-3P
      647020-24-4P 647020-25-5P 647020-26-6P
      647020-27-7P 647020-28-8P 647020-29-9P
      647020-30-2P 647020-31-3P 647020-32-4P
      647020-33-5P 647020-34-6P 647020-35-7P
      647020-36-8P 647020-37-9P 647020-38-0P
      647020-39-1P 647020-40-4P 647020-41-5P
      647020-42-6P 647020-43-7P 647020-44-8P
      647020-46-0P 647020-47-1P 647020-48-2P
      647020-49-3P 647020-50-6P 647020-51-7P
      647020-52-8P 647020-53-9P 647020-54-0P
      647020-55-1P 647020-56-2P 647020-57-3P
      647020-58-4P
        (preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent
        kinases)
IT
     647020-75-5P 647020-76-6P 647020-77-7P
      647020-80-2P 647020-81-3P 647020-82-4P
```

647020-89-1P

(preparation of pyrrolidinylchromenones as inhibitors of cyclin-dependent kinases)

=> d bib abs hitstr 166 2-3

L66 ANSWER 2 OF 3 USPATFULL on STN 89:12878 USPATFULL AN Therapeutically active flavonyl-1,4-dihydrophyridines TI IN Leonardi, Amedeo, Milan, Italy Pennini, Renzo, Milan, Italy Cazzulani, Pietro, Milan, Italy Nardi, Dante, Milan, Italy Recordati S.A., Chemical & Pharmaceutical Company, Chiasso, Switzerland PA (non-U.S. corporation) PΙ US 4806534 19890221 US 1986-921397 19861022 (6) ΑI IT 1985-22578 PRAI 19851022 DT Utility FS Granted EXNAM Primary Examiner: Fan, Jane T. Burns, Doane, Swecker & Mathis LREP CLMN Number of Claims: 61 Exemplary Claim: 1 ECL DRWN No Drawings LN.CNT 786 CAS INDEXING IS AVAILABLE FOR THIS PATENT. The novel flavonyl-1,4-dihydropyridines having the general formula (I): ##STR1## are therapeutically effective calcium antagonists and smooth muscle relaxant. CAS INDEXING IS AVAILABLE FOR THIS PATENT. IT 110714-79-9P (preparation of, as calcium antagonist and smooth muscle relaxant) RN 110714-79-9 USPATFULL CN3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(3-methyl-4-oxo-

2-phenyl-4H-1-benzopyran-8-yl)-, 2-(1H-imidazol-1-yl)ethyl methyl ester

$$\begin{array}{c|c}
\text{Me} & \text{H} & \text{Me} \\
\text{N} & \text{Me} & \text{O} \\
\text{C-O-CH}_2 - \text{CH}_2 - \text{N} \\
\text{N} & \text{N}
\end{array}$$

(9CI) (CA INDEX NAME)

L66 ANSWER 3 OF 3 USPATFULL on STN

AN 85:69647 USPATFULL

TI Circulation-active novel chromone- and thiochromone-substituted
 1,4-dihydropyridine-lactones

IN Goldmann, Siegfried, Wuppertal, Germany, Federal Republic of
 Bossert, Friedrich, Wuppertal, Germany, Federal Republic of
 Schramm, Matthias, Cologne, Germany, Federal Republic of
 Thomas, Gunter, Wuppertal, Germany, Federal Republic of
 Gross, Rainer, Wuppertal, Germany, Federal Republic of
 Bayer Aktiengesellschaft, Leverkusen, Germany, Federal Republic of
 (non-U.S. corporation)

PI US 4555512 19851126 AI US 1984-589614 19840314 (6) PRAI DE 1983-3311003 19830325

DT Utility FS Granted

EXNAM Primary Examiner: Michl, Paul R.; Assistant Examiner: Walker, Alex H.

LREP Sprung Horn Kramer & Woods

CLMN Number of Claims: 13 ECL Exemplary Claim: 1

DRWN No Drawings

LN.CNT 692

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Dihydropyridines of the formula ##STR1## in which R.sup.1, R.sup.2, R.sup.5 and R.sup.6 can be hydrogen or various halogen or organic radicals,

R.sup.4 is an optionally substituted hydrocarbon radical,

A is a direct bond, a C.sub.1 -C.sub.20 -alkylene chain or a C.sub.2 -C.sub.20 -alkenylene chain, which chains are optionally interrupted by O or S

X is O or S, and

Y is a direct bond, O, S, --NH--or--N-alkyl with 1 to 8 C atoms

or a pharmaceutically acceptable salt,

are useful as cardiotonic agents for improving heart contractility, antihypotonic agents, for lowering the blood sugar level, for detumescing mucous membranes and for influencing the salt and/or liquid balance.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 94127-70-5P

(preparation of)

RN 94127-70-5 USPATFULL

CN Furo[3,4-b]pyridine-3-carboxylic acid, 1,4,5,7-tetrahydro-2-methyl-5-oxo-4[4-oxo-2-(3-thienyl)-4H-1-benzopyran-8-yl]-, ethyl ester (9CI) (CA
INDEX NAME)

=> b home

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